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DYNAMIC FRACTURE IN BRITTLE MATERIALS

AFOSR GRANT #: F49620-03-1-0068

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Abstract

The primary objectives of this project were the formulation and analysis of canonical boundary value problems modeling dynamic fracture in brittle materials. The following issues concerning dynamic fracture in brittle were studied: unsteady, dynamic, mode I crack growth in linear elastic material; dynamic crack growth in functionally graded elastic bodies; dynamic, steady-state, generalized plane strain crack growth in anisotropic linear viscoelastic material; dynamic, transient, mode III crack growth in linear viscoelastic material. In addition to these problem areas, several new directions of research were initiated including various issues concerning finite deformations of nonlinear elastic bodies, the introduction of a new approach to incorporating molecular scale effects into continuum models of brittle fracture that avoids the logical inconsistencies inherent in classical linear elastic fracture mechanics and a novel approach to modeling residual stress accumulation in a continuously growing oxide layer on a metallic substrate. Among the issues investigated for finite deformations of hyperelastic material bodies are: the loss of strong ellipticity for hyperelastic materials characterized by the classical Fung strain energy function model and alternative strain energy characterizations that do not lose strong ellipticity; a study of various classes of large deformation solutions for the infinite elastic wedge problem that are unstable to small scale vibrational perturbations.

1 Objectives.

The primary objectives of this project were the formulation and analysis of canonical boundary value problems modeling dynamic fracture in brittle materials. The proposed objectives were to address the following problem areas.

1. **Unsteady Mode I Crack Growth in Elastic Material:** The P.I. proposed to generalize his previous analysis of the dynamic, transient growth of an antiplane shear crack in an infinite linear elastic body to the more difficult, but

physically more important, Mode I (opening mode) fracture setting. One of the goals of this line of research is to investigate the manner in which a macrocrack coalesces with a co-planar microcrack since there is considerable experimental evidence that this process plays a critical role in dynamic crack growth in brittle materials.

2. **Dynamic Crack Growth in Functionally Graded Elastic Bodies:** Functionally graded materials are becoming increasingly important in technological applications. However, few analyses of cracks in functionally graded material appearing in the literature have considered dynamic crack growth with realistic material properties. The P.I. proposed to generalize his work on dynamic crack growth in homogeneous elastic bodies to functionally graded material. Specifically, the P.I. proposed to consider the unsteady growth of a straight crack in a functionally graded material whose elastic properties vary both in the direction transverse to the crack plane and in the direction of crack propagation. The P.I. proposed to pursue an asymptotic approach initiated in his former AFOSR grant as a means of gaining insight into the boundary value problems corresponding to realistic material models. The P.I. proposed then use these asymptotic solutions to address the question of designing functionally graded materials with optimal fracture properties.
3. **Temperature Effects in Dynamic Crack Growth:** It has been observed experimentally in many materials that significant temperature increases occur within a thin neighborhood surrounding a dynamically propagating crack tip. Moreover the P.I. and his collaborator Francesco Costanzo have shown [1] within the context of the dynamic steady propagation of a semi-infinite anti-plane shear crack in an infinite linear elastic body that many of the experimentally observed dynamic fracture phenomena that seem to run counter to classical linear elastic fracture mechanics predictions follow naturally from modeling the crack tip region by a temperature sensitive cohesive zone. The P.I. proposed to extend this work to the opening mode (mode I) fracture setting. Two approaches were to be pursued. The first is to generalize the combined analytical/numerical methods used previously on the mode III problem to mode I context, and the second is to assist Dr. Costanzo's project to develop a direct numerical simulation scheme based upon a discontinuous Galerkin methodology that he has been pursuing to treat general elastodynamic problems with moving singularities.
4. **Dynamic Crack Growth in Viscoelastic Bodies:** Fiber reinforced composites have myriad uses as structural materials in Air Force applications as well as everyday life. Understanding the fracture behavior of such materials is of paramount importance. Many fiber reinforced composites utilize polymeric binders which exhibit considerable hysteresis under cyclic loading. The P.I. proposed to study the dynamic steady-state problem of a semi-infinite crack propagating in an infinite anisotropic viscoelastic body under generalized plane strain deformations with fully mixed mode loading (combined modes I, II and

III). The viscoelasticity is intended to model a polymeric binder matrix while the anisotropy models fiber orientation.

2 Accomplishments.

Progress was made on the proposed problem areas as well as in two new directions begun during the grant period but not part of the originally proposed work. Results from all of the problem areas are summarized below.

2.1 Unsteady Mode I Crack Growth in Elastic Material.

The P.I. and Dr. Tanya Leise, Amherst College, have recently initiated the analysis of the titled problem. To date they have carried out the key step of constructing the Dirichlet-to-Neumann map required to relate the crack opening displacement to the driving tractions for a semi-infinite, Mode I crack in an infinite, linearly elastic body. The crack tip is allowed to accelerate arbitrarily. They are now applying this Dirichlet-to-Neumann map to the consideration of a crack tip cohesive zone and use of the critical crack opening displacement fracture criterion for the prediction of the crack tip motion. They expect to have a code for performing crack growth simulations based upon this analysis implemented within six months time. This work generalizes the corresponding analysis of the mode III problem presented in [2, 3].

2.2 Dynamic Crack Growth in Functionally Graded Elastic Bodies.

The P.I. and his former student, David Zeigler (Postdoc at Sandia, Livermore and now Asst. Prof. at Cal. State Sacramento) considered the problem of dynamic crack growth along an interface in a functionally graded composite material. In such a material, the constitutive properties vary smoothly away from a bi-material interface. Such composite material systems are of increasing importance in technological applications since they offer the prospect of creating laminated composite materials that are not susceptible to the debonding failure occurring at traditional bi-material interfaces due to the mismatch in material properties. They studied the problem of a semi-infinite, anti-plane shear crack propagating dynamically along an interface between two half-planes of linear elastic material with shear modulus varying spatially in the direction transverse to the fracture plane. The mathematical difficulty stems from the fact that elastic waves are dispersive in such a medium due to the spatial dependence of the sound speed in the bulk material. To study this problem, they performed an asymptotic analysis based upon the assumption that the material

properties through out the bulk material are given by an asymptotic series with zero order term corresponding to a homogeneous elastic material.

Since there are almost no analytical solutions to dynamic, unsteady crack problems in nonhomogeneous elastic material available in the literature against which to check the range of validity of the asymptotic solution described above, Zeigler and the P.I. applied their asymptotic approach to the simpler quasi-static problem for which one can construct analytic solutions for a few special classes of nonhomogeneous material models. Numerical results show quite reasonable agreement between the asymptotic approximation to the Stress Intensity Factor (SIF) and the true SIF for this quasi-static problem. This work has not yet been submitted for publication.

2.3 Dynamic Crack Growth in Viscoelastic Material.

The work on modeling dynamic crack growth in viscoelastic material considered two classes of problems: dynamic, steady-state, generalized plane strain (coupled Modes I, II, III) crack growth in anisotropic, linear viscoelastic material; dynamic, unsteady, anti-plane shear (Mode III) in isotropic linear viscoelastic material.

2.3.1 Dynamic, Steady-State, Generalized Plane Strain Crack Growth in Anisotropic Linear Viscoelastic Material.

The P.I. initiated a study of dynamic, steady-state crack problems in a general, linear anisotropic viscoelastic body. The intended application is to composite materials whose material properties can be approximated by those of a homogeneous material exhibiting anisotropy and hysteresis under cyclic loading. While some analytical studies exist in the literature (or in pre-print form) of dynamic steady-state crack propagation in an anisotropic elastic material, the corresponding viscoelastic problem has not been addressed. This is due partly to the fact that the approach developed by Stroh that has been the basis for nearly all existing analytical work on the elastic problem, does not generalize to the viscoelastic case.

The P.I. has developed a general solution method based upon transform and complex variable techniques that produces a full field solution to a semi-infinite crack problem under general crack face loadings leading to generalized plane strain deformations. A key step in the analysis is the construction of the Dirichlet-to-Neumann map on the bounding plane for an anisotropic viscoelastic half-space under dynamic steady-state conditions.

Two classes of crack face tractions were simulated: a point load placed a prescribed distance behind the crack tip and a uniform traction applied over a finite interval placed a prescribed distance behind the crack tip. They each exhibited the surprising

feature of the Stress Intensity Factor (SIF) vanishing at a crack speed strictly less than the glassy Rayleigh wave speed. The P.I. proved that if the loading interval begins at the crack tip, then the SIF cannot vanish until the glassy Rayleigh wave speed, but if moved back from the crack tip, then it can. This offers an explanation of the famous experimental observations of Ravi-Chandar and Knauss from the early 1980s of cracks dynamically propagating in brittle polymers that cracks (in brittle polymers) quickly reached a constant speed of propagation that was about 40%-60% of the glassy Rayleigh wave speed. A dynamic elastic analysis predicts that cracks should accelerate up to the glassy Rayleigh wave speed. Their loading was uniform on a compact interval beginning a short distance behind the crack tip. As the crack begins to run, the loading distance recedes farther from the crack tip. While their experiment is transient, the dynamic, steady-state analysis described above suggests that maximum crack speeds should be around the equilibrium shear wave speed, which is within the range of speeds they observed. It should be emphasized that this behavior is not predicted by a dynamic elastic analysis nor observed in the corresponding mode III dynamic viscoelastic setting. This work is contained in [4].

2.3.2 Dynamic, Transient, Mode III Crack Growth in Linear Viscoelastic Material.

The P.I. along with T. Leise generalized their method for solving dynamic unsteady crack problems in an isotropic linear elastic body to a viscoelastic body [5, 6]. Previously they had applied their approach to studying multiple co-planar cracks in order to simulate the growth and coalescence of a system of (anti-plane shear) micro-cracks with a main macro-crack. Such growth and coalescence of micro-cracks is thought to be a common mechanism by which macro-cracks grow in brittle materials. They applied their approach to a single semi-infinite anti-plane shear crack in a viscoelastic body. This solution is the first dynamic, unsteady crack analysis valid for a general linear viscoelastic body, and their simulations demonstrate clearly the critical role played by material viscoelasticity in controlling the speed of a propagating crack. In particular, not accounting for viscoelasticity in the material can easily lead to errors in excess of 100% in predictions of distances a crack tip will propagate for a given loading and glassy (elastic), material properties.

2.4 Finite Elastic Deformations.

The P.I. began a mathematical investigation of the large deformation behavior of rubbery materials. The setting is finite elasticity and two themes are being pursued: the convexity or strong ellipticity properties of anisotropic finite elastic constitutive models; the stability of various classes of solutions to finite elastic boundary value problems for a wedge shaped body.

2.4.1 Strong Ellipticity for Hyperelastic Material Models.

The P.I. and his former postdoc Patrick Wilber (currently Asst. Prof. Univ. of Akron) showed that the classical anisotropic hyperelastic constitutive model due to Y. C. Fung fails to be strongly elliptic at any finite deformation. They also examined various approaches to modeling anisotropic finite elastic behavior through which strong ellipticity or convexity properties can be guaranteed. These results, which are contained in the two papers [7, 8], have important implications for modeling material behavior and for doing numerical computations.

Subsequently, the P.I. and his graduate student, Tsvetanka Sendova, extended this work of Walton and Wilber. In the most recent work, the strain energy function is assumed to be a function of the novel set of invariants of the Hencky strain tensor introduced by Criscione, Humphrey, Douglas and Hunter in 2000.

While convenient for checking conditions such as strong ellipticity, the standard formulation of hyperelasticity is ill suited for the experimental characterization of real material because the standard list of invariants are highly correlated. As a consequence, Criscione et al proposed a model for the strain energy function of an isotropic hyperelastic material that is formulated in terms of a novel set of invariants of the Hencky strain (also called the logarithmic or "natural" strain). These invariants were shown to have a certain orthogonality property that makes models based upon them ideal for fitting experimental data. Moreover, these new invariants have direct physical interpretation as volumetric expansion, the magnitude of distortion and the mode of distortion, which the standard list of invariants fail to have.

On the negative side, for a hyperelastic material model based upon Criscione's invariants of the Hencky strain, determining conditions characterizing strong ellipticity is very much more complicated than for models based upon the standard list of invariants of the left Cauchy-Green strain. Criscione and Wilber recently derived conditions guaranteeing the satisfaction of the Baker-Ericksen inequalities for Criscione's formulation of isotropic hyperelastic material, but this lends no help to characterizing strong ellipticity. The primary impediments to deriving constitutive restrictions for Criscione's model based upon strong ellipticity are having a convenient expression for the Fréchet derivative of the logarithmic strain with respect to the deformation gradient and the complicated functional form of gradients of Criscione's invariants. In [9], the P.I. and his student Tsvetanka Sendova showed how to overcome the first impediment and made progress on the latter. Specifically, the desired convenient expression for the Fréchet derivative of the logarithmic strain with respect to the deformation gradient was derived and partial results on strong ellipticity were developed using that Fréchet derivative.

2.4.2 Stability of Finite Deformations in Hyperelastic Material.

The P.I. demonstrated in [10] that several classes of plane strain, large deformation solutions for the infinite elastic wedge problem are unstable to small scale vibrational perturbations. He also showed that this property is a nonlinear elastic effect that does not occur for the linear elastic approximation. Subsequently, he and P. Wilber studied the issue of solutions to the wedge problem with uniformly bounded stresses. A number of previous researchers had shown that a certain class of homogeneous deformations lead to bounded stresses, and they exhibited a few classes of nonhomogeneous deformations exhibiting stress singularities at the wedge apex. The P.I. and Wilber showed [11] that even among a very wide class of fully three dimensional nonhomogeneous deformations, none exist with bounded stresses at the apex; only homogeneous deformations can lead to bounded stresses. These results have implications for predicting the behavior of rubbery shock absorbers.

2.5 Incorporating Molecular Scale Phenomena into Continuum Fracture Models.

The physics of interfaces has a long and rich history. While it is three-dimensional on an atomic scale, it is usually represented as a two-dimensional dividing surface on a continuum scale. As this dividing surface is approached from either side, the intermolecular forces and the material behaviors of the adjoining phases are altered as a result of the discontinuity in the intermolecular force fields. When the adjoining phases are "semi-infinite (more than 100 nm thick), this discontinuity can be accounted for by attributing a surface energy (or surface tension) to the interface.

An important setting for these considerations is thin films, such as the thin film formed between fracture faces near the tip of a fracture or the thin films of silicon dioxide or semiconductors employed in electronic chips. Material within or in the immediate neighborhood of thin films is subjected to intermolecular forces from at least three phases. These effects can no longer be taken into account by simply adding one or more interfacial tensions. J. C. Slattery (Texas A&M Univ.) and colleagues recently showed how these effects can be taken into account in continuum mechanics through the introduction of mutual forces based upon intermolecular potentials.

A wide range of important mechanics/materials issues involving interfacial phenomena can be addressed through the proposed theoretical paradigm. Among these are: fracture of a single component material, interfacial fracture or debonding of a composite material body, stability of an ultra-thin solid film on a solid substrate (e.g. silicon dioxide/silicon composite). All of these problem areas share essential modeling ingredients: correction of bulk material (continuum level) constitutive description near an interface due the close proximity of one or more neighboring phases of dissimilar material, ab initio calculations at atomistic/molecular scales to determine the contin-

uum correction term for each particular material system. Oh, Slattery and Walton [12] applied these ideas to a new modeling paradigm for brittle fracture. Among the important observations of that paper is that incorporation of intermolecular force corrections to bulk material behavior near a fracture surface results in predictions of a smoothly closing crack tip, in stark contrast to classical linear elastic fracture mechanics. While this observation comes via numerical simulation in [12], it has been recently demonstrated rigorously by the P.I and his student T. Sendova. This latter result is part of work in progress by Sendova and the P.I. on various analytical issues arising from this novel approach to brittle fracture.

2.6 Predicting Stress Evolution During Oxidation of a Metal.

The oxidation behavior of metals has been extensively studied since it plays important roles in modern technology. For example, the oxidation of silicon is one of the critical steps in the fabrication of semiconductor devices; the oxide becomes a barrier to dopant diffusion into the semiconductor substrate. Also the life of titanium metal matrix composites may be significantly reduced at high temperatures, since oxides of titanium that form are relatively brittle and prone to fracture. Stress analysis in oxidation problems usually follows the approach of introducing a known eigenstrain in the constitutive equation for elastic stress-deformation behavior in the oxide. The eigenstrain is assumed to be independent of time and position; it is the strain that would be observed in an imaginary stress-free phase transformation. The total strain of the oxide is the sum of elastic strain and this eigenstrain. As shown in [13], the principal problem with the eigenstrain approach is that the current or deformed configuration implied by the eigenstrain is incompatible with the current configuration that results from the solution of the diffusion/reaction problem modeling oxidation. In addition, for oxidation of most metals, the eigenstrain approach often grossly over estimates the stresses. In the present approach, the diffusion/reaction problem is solved simultaneously with the momentum balance formulated in the current configuration via a paradigm that avoids introducing an ad hoc eigenstrain. Results are illustrated for oxidation of silicon.

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